

# STN-Structure Search

6-18-05

10/644,981

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L4 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:412819 CAPLUS  
 DOCUMENT NUMBER: 140:423713  
 TITLE: Preparation of benzodiazepine derivatives for the treatment of diabetes mellitus  
 INVENTOR(S): Yu, Jinghua; Ghosh, Soumitra S.; Pei, Yazhong  
 PATENT ASSIGNEE(S): Mitokor, Inc., USA  
 SOURCE: PCT Int. Appl., 64 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041286	A1	20040521	WO 2003-US34340	20031027
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:

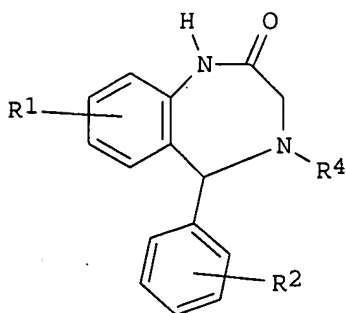
US 2002-422591P

P 20021030

OTHER SOURCE(S):

MARPAT 140:423713

GI



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AB The invention provides compns. and methods for altering insulin secretion using a benzodiazepine compound that inhibits calcium efflux via the mitochondrial calcium/ sodium antiporter (MCA). The title compds., e.g. I [R1, R2 = halo; R4 = (un)substituted alkyl, etc.; a provision is given], are prepared. Methods of treatment are thereby provided, and are particularly useful for treatment of subjects having, or suspected of being at risk for having, diabetes mellitus. The bioactivities of compds. of this invention were demonstrated.

IT 690999-62-3P 690999-64-5P

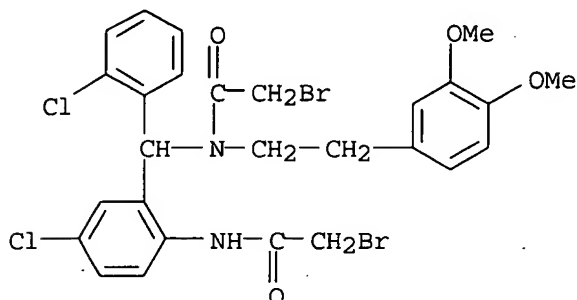
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzodiazepine derivs. for the treatment of diabetes mellitus)

RN 690999-62-3 CAPLUS

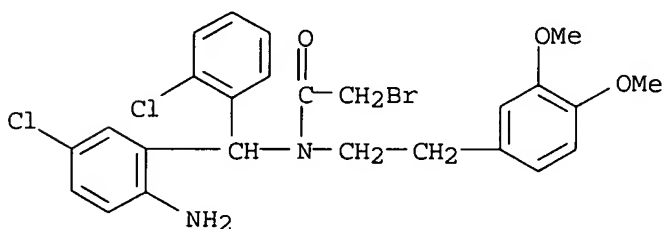
10/644,981

CN Acetamide, 2-bromo-N-[[2-[(bromoacetyl)amino]-5-chlorophenyl](2-chlorophenyl)methyl]-N-[2-(3,4-dimethoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)



RN 690999-64-5 CAPLUS

CN Acetamide, N-[(2-amino-5-chlorophenyl)(2-chlorophenyl)methyl]-2-bromo-N-[2-(3,4-dimethoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:669869 CAPLUS

DOCUMENT NUMBER: 137:352486

TITLE: Asymmetric Carbon-Carbon Bond Formations in Conjugate Additions of Lithiated N-Boc Allylic and Benzylic Amines to Nitroalkenes: Enantioselective Synthesis of Substituted Piperidines, Pyrrolidines, and Pyrimidinones

AUTHOR(S): Johnson, Timothy A.; Jang, Doo Ok; Slafer, Brian W.; Curtis, Michael D.; Beak, Peter

CORPORATE SOURCE: Department of Chemistry, Roger Adams Laboratory, University of Illinois, Urbana, IL, 61801, USA

SOURCE: Journal of the American Chemical Society (2002), 124(39), 11689-11698

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB (-)-Sparteine mediated lithiations of N-Boc-allylic and benzylic amines provide configurationally stable intermediates which on conjugate addns. to nitroalkenes provide highly enantioenriched enecarbamate products in good yields, and with high diastereoselectivities. Straightforward transformations of these adducts offer general routes to substituted 3,4-substituted piperidines, 3,4-substituted pyrrolidines, and 4,5-substituted pyrimidinones. Diastereoselective substitutions of intermediate lactams followed by reduction provide 3,4,5-substituted piperidines and 3,4-trisubstituted pyrrolidines. Lithiation adjacent to nitrogen of 3,4-substituted piperidines and pyrrolidines followed by

diastereoselective substitution opens a route to 2,4,5- and 2,4,5,6-substituted piperidines as well as 2,3,4- and 2,3,4,5-substituted pyrrolidines. The enantiomers of the enecarbamate and 3,4-substituted piperidine products may be accessed by stannylation/transmetalation sequences as well as by further manipulation of 4-substituted piperidones. The methodol. is used to synthesize both enantiomers of an aspartic peptidase inhibitor intermediate, 3-hydroxy-4-phenylpiperidine, as well as the antidepressant (+)-femoxetine.

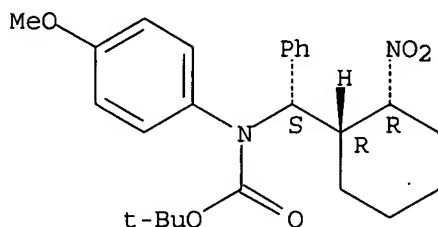
IT 474924-82-8P 474925-58-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(asym. carbon-carbon bond formations in conjugate addns. of lithiated N-Boc allylic and benzylic amines to nitroalkenes)

RN 474924-82-8 CAPLUS

CN Carbamic acid, (4-methoxyphenyl)[(S)-[(1R,2R)-2-nitrocyclohexyl]phenylmethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

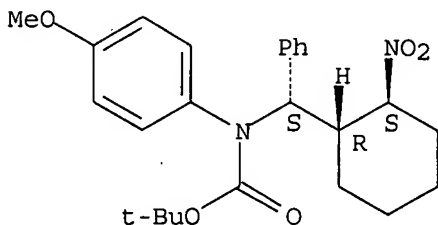
Absolute stereochemistry.



RN 474925-58-1 CAPLUS

CN Carbamic acid, (4-methoxyphenyl)[(S)-[(1R,2S)-2-nitrocyclohexyl]phenylmethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

47

THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:658081 CAPLUS

DOCUMENT NUMBER: 137:185493

TITLE: Preparation of 1,3-diaminopropanes as analgesics

INVENTOR(S): Sundermann, Bernd; Buschmann, Helmut; Koegel, Babette-Yvonne; Merla, Beatrix; Risch, Nikolaus

PATENT ASSIGNEE(S): Gruenenthal G.m.b.H., Germany

SOURCE: PCT Int. Appl., 92 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

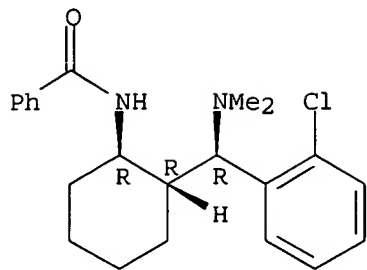
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002066432	A1	20020829	WO 2002-EP1765	20020220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10108307	A1	20020829	DE 2001-10108307	20010221
CA 2438704	AA	20020829	CA 2002-2438704	20020220
EP 1363885	A1	20031126	EP 2002-714169	20020220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002007535	A	20040309	BR 2002-7535	20020220
JP 2005503330	T2	20050203	JP 2002-565949	20020220
NO 2003003697	A	20031017	NO 2003-3697	20030820
US 2004067928	A1	20040408	US 2003-644981	20030821
ZA 2003007321	A	20050110	ZA 2003-7321	20030918
PRIORITY APPLN. INFO.:			DE 2001-10108307	A 20010221
			WO 2002-EP1765	W 20020220
AB	R2(NR3R4)CHR1CHCH(NR5R6)A [I; R1 = alkyl, cycloalkyl, alkylcycloalkyl, aryl; R2 - alkyl, cycloalkyl, aryl, alkylcycloalkyl, alkylaryl, heterocyclyl, alkylheterocyclyl; whereby R1 and R2 can not be together aryl and heterocyclyl, or R1R2 = (substituted) (benzocondensed) (CH2)m; m = 2-6; R3 = H, alkyl, cycloalkyl, alkylcycloalkyl, alkylaryl, heterocyclyl, alkylheterocyclyl, COR7; or R3R4 = (substituted) (CH2)n, (CH2)2X(CH2)2; n = 3-7; X = O, S, NR8; R5, R6 = alkyl, cycloalkyl, aryl, alkylcycloalkyl, alkylaryl; or R5R6 = (substituted) (CH2)o, (CH2)2Y(CH2)2; Y = O, S, NR9; o = 3-7; A = aryl, heteroaryl, CO2R10, 2-propyl; R7 = alkyl, cycloalkyl, aryl, heterocyclyl, alkylcycloalkyl, alkylaryl, alkylheterocyclyl; R8, R9 = H, alkyl, cycloalkyl, aryl, alkylcycloalkyl, alkylaryl, heterocyclyl; R10 = alkyl, cycloalkyl, aryl, alkylcycloalkyl, alkylaryl], were prepared as racemate or in the form of diastereomers or enantiomers. Tested I at 10 mg/kg i.v. in mice gave 34-85% phenylquinone-induced Writhing.			
IT	187463-24-7P 452093-15-1P 452093-27-5P 452093-30-0P 452093-35-5P 452093-38-8P 452093-42-4P 452093-45-7P 452093-47-9P 452093-51-5P 452093-55-9P 452093-58-2P 452093-64-0P 452093-70-8P 452093-75-3P 452093-80-0P 452093-84-4P 452093-90-2P 452093-94-6P 452093-97-9P 452093-99-1P 452094-01-8P 452094-03-0P 452094-05-2P 452094-07-4P 452094-09-6P 452094-12-1P 452094-16-5P 452094-19-8P 452094-23-4P 452094-28-9P 452094-34-7P 452094-37-0P 452094-40-5P 452094-46-1P 452094-52-9P 452094-58-5P 452094-61-0P 452094-64-3P 452094-67-6P 452094-70-1P 452094-73-4P 452094-76-7P 452094-79-0P 452094-86-9P 452094-91-6P 452094-94-9P 452094-97-2P 452095-00-0P 452095-03-3P 452095-06-6P 452095-09-9P 452095-12-4P 452095-15-7P 452095-20-4P 452095-24-8P 452095-28-2P 452095-31-7P 452095-33-9P 452095-35-1P 452095-37-3P 452095-39-5P 452095-41-9P 452095-43-1P 452095-45-3P 452095-48-6P			

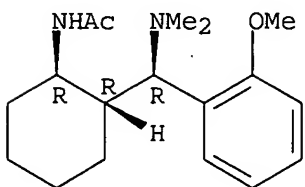
10/644,981



RN 452095-70-4 CAPLUS

CN Acetamide, N-[(1R,2R)-2-[(R)-(dimethylamino)(2-methoxyphenyl)methyl]cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

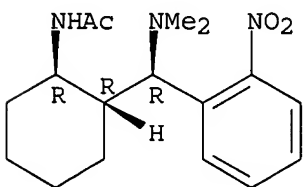
Relative stereochemistry.



RN 452095-71-5 CAPLUS

CN Acetamide, N-[(1R,2R)-2-[(R)-(dimethylamino)(2-nitrophenyl)methyl]cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

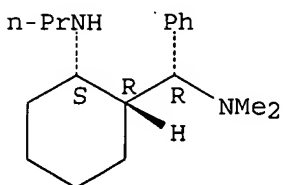
Relative stereochemistry.



RN 452095-74-8 CAPLUS

CN Benzenemethanamine, N,N-dimethyl- $\alpha$ -[(1R,2S)-2-(propylamino)cyclohexyl]-, ( $\alpha$ R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

*Answers*

10/644,981

ACCESSION NUMBER: 2002:619639 CAPLUS  
DOCUMENT NUMBER: 138:89325  
TITLE: Efficient synthesis of diastereomerically pure  
1,3-diamines  
AUTHOR(S): Merla, Beatrix; Risch, Nikolaus  
CORPORATE SOURCE: Fachbereich Chemie und Chemietechnik, Universitat  
Paderborn, Paderborn, 33098, Germany  
SOURCE: Synthesis (2002), (10), 1365-1372  
CODEN: SYNTBF; ISSN: 0039-7881  
PUBLISHER: Georg Thieme Verlag  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 138:89325

AB The regio- and diastereoselective synthesis of 1,3-diamines using  
inexpensive starting materials is described.  $\beta$ -Aminoketones are  
easily transformed diastereoselectively into syn, anti-, anti, anti-, or  
anti, syn-1,3-diamines using different methodologies. The configuration  
of the products was determined by NMR.

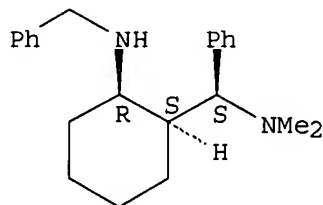
IT 187463-24-7P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(deprotection of; preparation of regio- and diastereomerically pure diamines  
from corresponding aminoketones and their configuration)

RN 187463-24-7 CAPLUS

CN Benzenemethanamine, N,N-dimethyl- $\alpha$ -[(1R,2S)-2-  
[(phenylmethyl)amino]cyclohexyl]-, ( $\alpha$ R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 452093-15-1P 452093-27-5P 452093-30-0P

452093-35-5P 452093-38-8P 452093-42-4P

452093-45-7P 452093-47-9P 452093-51-5P

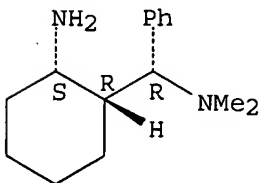
452093-55-9P 452093-58-2P 452093-64-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation of regio- and diastereomerically pure diamines from  
corresponding aminoketones and their configuration)

RN 452093-15-1 CAPLUS

CN Benzenemethanamine,  $\alpha$ -[(1R,2S)-2-aminocyclohexyl]-N,N-dimethyl-,  
( $\alpha$ R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 452093-27-5 CAPLUS

CN Benzenemethanamine,  $\alpha$ -[(1R,2S)-2-aminocyclohexyl]-2-chloro-N,N-

10/644,981

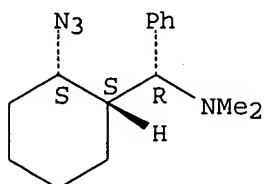
(reduction of; preparation of regio- and diastereomerically pure diamines from

corresponding aminoketones and their configuration)

RN 485403-30-3 CAPLUS

CN Benzenemethanamine,  $\alpha$ -[(1R,2R)-2-azidocyclohexyl]-N,N-dimethyl-, ( $\alpha$ S)-rel- (9CI) (CA INDEX NAME)

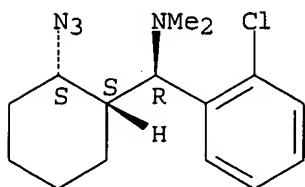
Relative stereochemistry.



RN 485403-31-4 CAPLUS

CN Benzenemethanamine,  $\alpha$ -[(1R,2R)-2-azidocyclohexyl]-2-chloro-N,N-dimethyl-, ( $\alpha$ S)-rel- (9CI) (CA INDEX NAME)

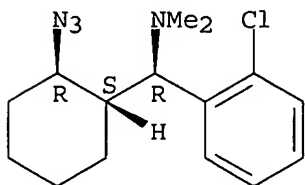
Relative stereochemistry.



RN 485403-32-5 CAPLUS

CN Benzenemethanamine,  $\alpha$ -[(1R,2S)-2-azidocyclohexyl]-2-chloro-N,N-dimethyl-, ( $\alpha$ S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:634954 CAPLUS

DOCUMENT NUMBER: 133:218841

TITLE: Mixed herbicide compositions

INVENTOR(S): Kobayashi, Kazunori; Ono, Yoshimasa; Miyazawa, Takeshige

PATENT ASSIGNEE(S): Kumiai Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

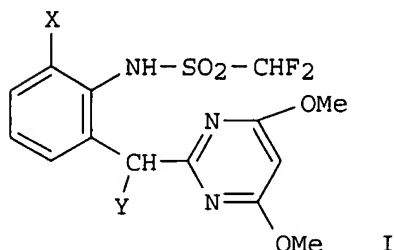
LANGUAGE: Japanese

10/644,981

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000247814	A2	20000912	JP 1999-53557	19990302
PRIORITY APPLN. INFO.:			JP 1999-53557	19990302
OTHER SOURCE(S):	MARPAT 133:218841			
GI				



AB Mixed herbicides active for a long period, controlling weeds such as barnyard grass, after a single application to flooded rice paddies, are presented. Sulfonyl anilide derivative of I, where X = alkoxyalkyl; Y = alkylamino, in combination with the following compds., namely, 2-chloro-2',6'-diethyl-N-(n-propoxyethyl)-acetanilide, N-butoxymethyl-2-chloro-2',6'-dimethylacetanilide, 2-[4-(2',4'-dichloro-m-toluoxy)-1,3-dimethylpyrazole-5-yloxy]-4-Me acetophenone, 2-(2,4-dichloro-3-methylphenoxy)propionic anilide, 2-bromo-N-( $\alpha,\alpha$ -dimethylbenzyl)-3,3-dimethyl-butylamide or 3-(4-chloro-5-cyclopentyl-oxy-2-fluorophenyl)-5-isopropylidene-1,3-oxazolidine-2,4-dione are claimed.

IT 291291-31-1 291291-32-2 291291-33-3  
291291-34-4 291291-35-5 291291-36-6  
291291-38-8 291291-42-4 291291-47-9  
291291-48-0

RL: AGR (Agricultural use); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process); USES (Uses) (mixed sulfonylanilide herbicide compns.)

RN 291291-31-1 CAPLUS

CN Acetamide, 2-chloro-N-(2,6-diethylphenyl)-N-(2-propoxyethyl)-, mixt. with N-[2-[(diethylamino)(4,6-dimethoxy-2-pyrimidinyl)methyl]-6-(methoxymethyl)phenyl]-1,1-difluoromethanesulfonamide (9CI) (CA INDEX NAME)

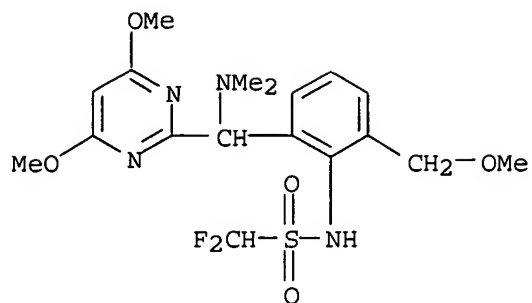
CM 1

CRN 221204-49-5

CMF C20 H28 F2 N4 O5 S



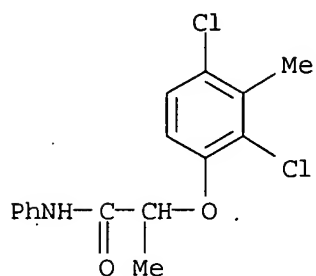
10/644,981



CM 2

CRN 84496-56-0

CMF C16 H15 Cl2 N O2



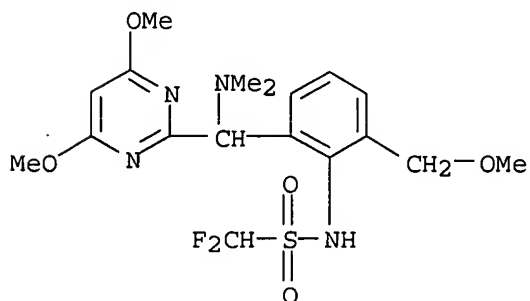
RN 291291-48-0 CAPLUS

CN Butanamide, 2-bromo-3,3-dimethyl-N-(1-methyl-1-phenylethyl)-, mixt. with N-[2-[(4,6-dimethoxy-2-pyrimidinyl)(dimethylamino)methyl]-6-(methoxymethyl)phenyl]-1,1-difluoromethanesulfonamide (9CI) (CA INDEX NAME)

CM 1

CRN 221204-54-2

CMF C18 H24 F2 N4 O5 S

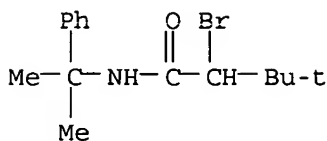


CM 2

CRN 74712-19-9

10/644,981

CMF C15 H22 Br N O



L4 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:147774 CAPLUS

DOCUMENT NUMBER: 130:223289

TITLE: Preparation of sulfonanilide moiety containing pyrimidine derivatives as herbicides

INVENTOR(S): Yoshimura, Isao; Miyazaki, Masahiro; Suzuki, Senji; Nakaya, Masao; Tamaru, Masatoshi; Ono, Yoshimasa; Ida, Tomohisa; Yanagisawa, Katsutada; Sadohara, Hideo

PATENT ASSIGNEE(S): Kumiai Chemical Industry Co., Ltd., Japan; Ihara Chemical Industry Co., Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 57 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

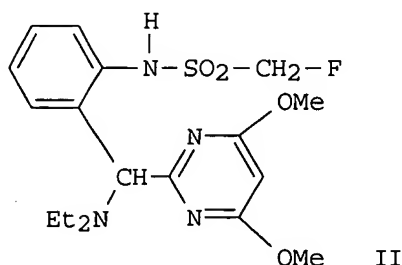
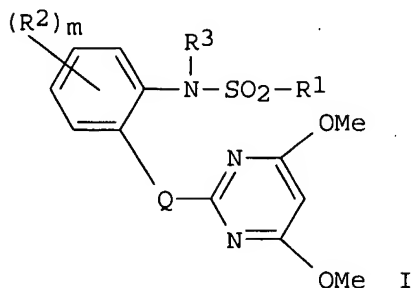
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11060562	A2	19990302	JP 1998-173980	19980605
PRIORITY APPLN. INFO.:			JP 1997-169454	A 19970611
OTHER SOURCE(S):	MARPAT	130:223289		

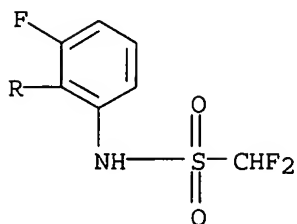
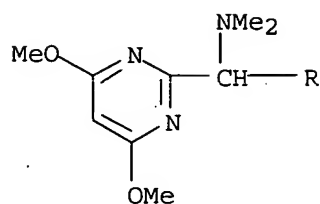
GI



AB The title compds. I [R1 = (un)substituted alkyl, etc.; R2 = H, halo, etc.; R3 = H, alkyl, etc.; Q = CH(NR4R5), etc.; m = 1 -4; R4, R5 = H, alkyl, etc.] are prepared The title compound II (at 100 g/10 are) gave  $\geq 90\%$  control of Scirpus juncoides.

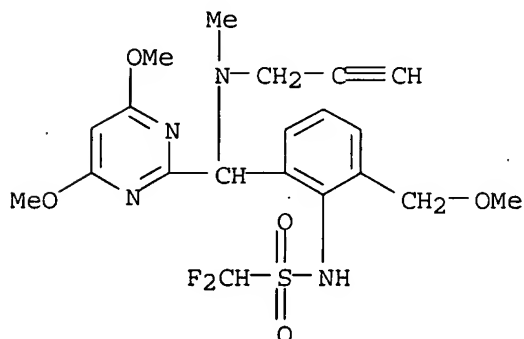
IT 221203-43-6P 221203-44-7P 221203-45-8P  
221203-48-1P 221203-49-2P 221203-50-5P  
221203-51-6P 221203-52-7P 221203-53-8P  
221203-54-9P 221203-55-0P 221203-56-1P  
221203-57-2P 221203-58-3P 221203-59-4P  
221203-60-7P 221203-61-8P 221203-91-4P  
221203-95-8P 221203-96-9P 221203-97-0P  
221203-98-1P 221203-99-2P 221204-00-8P  
221204-01-9P 221204-02-0P 221204-27-9P

10/644,981



RN 221205-66-9 CAPLUS

CN Methanesulfonamide, N-[2-[(4,6-dimethoxy-2-pyrimidinyl)(methyl-2-propynylamino)methyl]-6-(methoxymethyl)phenyl]-1,1-difluoro- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:355784 CAPLUS

DOCUMENT NUMBER: 129:136152

TITLE: N-phenyl-1-aza-2-cyano-1,3-butadienes: an intramolecular hetero Diels-Alder strategy for the construction of 1,4-benzodiazepines

AUTHOR(S): Goulaouic-Dubois, Catherine; Adams, David R.; Sisti, Nicholas J.; Fowler, Frank W.; Grierson, David S.

CORPORATE SOURCE: Inst. Chimie Substances Naturelles, CNRS, Gif-sur-Yvette, 91198, Fr.

SOURCE: Tetrahedron Letters (1998), 39(24), 4283-4286  
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:136152

AB A new approach to the construction of tricyclic 1,4-benzodiazepines was developed, based upon the intramol. Diels-Alder reaction of 2-cyano-1-azadienes [i.e., [2-[2-[(2-propenylamino)methyl]phenyl]imino]-3-butenenitriles]. This study revealed the difficulties inherent to the direct transformation of an imine-amide to an azadiene, but demonstrated

the efficiency of the intramol. [4+2] cycloaddn. of azadienes as a means to access benzodiazepines. The target compound was 3,4,4a,5-tetrahydro-7-phenylpyrido[1,2-a][1,4]benzodiazepine-1-carbonitrile.

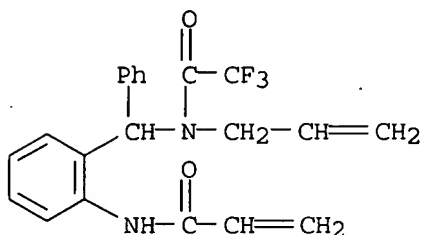
IT 210534-47-7P 210534-48-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of phenylpyridobenzodiazepinecarbonitrile via Diels-Alder reaction of [[(propenylamino)methyl]phenylimino]butenenitrile)

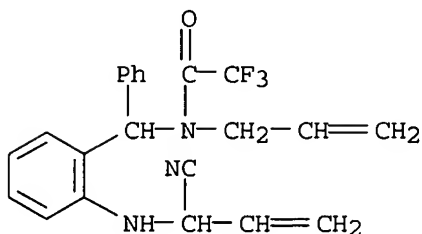
RN 210534-47-7 CAPLUS

CN 2-Propenamide, N-[2-[phenyl[2-propenyl(trifluoroacetyl)amino)methyl]phenyl]- (9CI) (CA INDEX NAME)



RN 210534-48-8 CAPLUS

CN Acetamide, N-[[2-[(1-cyano-2-propenyl)amino]phenyl]phenylmethyl]-2,2,2-trifluoro-N-2-propenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:129715 CAPLUS

DOCUMENT NUMBER: 126:186041

TITLE: A simple and highly diastereoselective one-pot synthesis of 1,3-diamines

AUTHOR(S): Merla, Beatrix; Arend, Michael; Risch, Nikolaus

CORPORATE SOURCE: Fachbereich Chemie Chemietechnik, Universitaet-Gesamthochschule Paderborn, Paderborn, D-33098, Germany

SOURCE: Synlett (1997), (2), 177-178  
CODEN: SYNLES; ISSN: 0936-5214

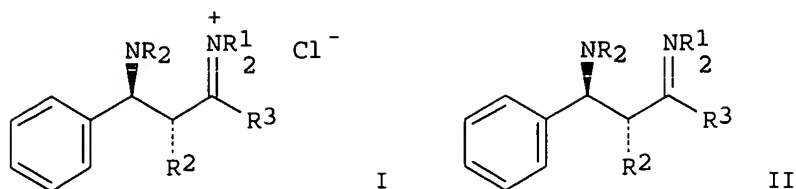
PUBLISHER: Thieme

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 126:186041

GI



AB A convenient 1-pot procedure for the highly diastereoselective synthesis of 1,3-diamines from inexpensive starting materials is described. Enamines (E)-R<sup>2</sup>CH:CR<sup>3</sup>NR<sup>1</sup><sub>2</sub> [R<sup>1</sup><sub>2</sub> = (CH<sub>2</sub>)<sub>4</sub>, R<sup>2</sup>R<sup>3</sup> = (CH<sub>2</sub>)<sub>4</sub> or R<sup>2</sup> = Me, R<sup>3</sup> = Ph; R<sup>1</sup><sub>2</sub> = (CH<sub>2</sub>)<sub>2</sub>O(CH<sub>2</sub>)<sub>2</sub>, R<sup>2</sup>R<sup>3</sup> = (CH<sub>2</sub>)<sub>4</sub> or R<sup>2</sup> = Me, R<sup>3</sup> = Ph, Et; R<sup>1</sup> = Et, R<sup>2</sup> = Me, R<sup>3</sup> = Ph] are aminoalkylated with preformed [PhCH:N+R<sup>2</sup>]Cl<sup>-</sup> [R = Me; R<sup>2</sup> = (CH<sub>2</sub>)<sub>4</sub>, (CH<sub>2</sub>)<sub>2</sub>O(CH<sub>2</sub>)<sub>2</sub>, (CH<sub>2</sub>)<sub>5</sub>] yielding exclusively the corresponding quaternary iminium salts I. In-situ reduction of the latter with NaBH<sub>4</sub>/MeOH provides a broad access to the corresponding 1,3-diamines II in 42-85% yield.

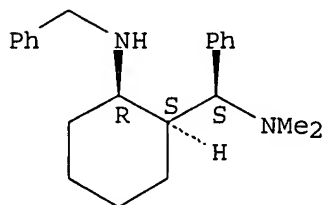
IT **187463-24-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(stereoselective synthesis of diamines)

RN 187463-24-7 CAPLUS

CN Benzenemethanamine, N,N-dimethyl-α-[(1R,2S)-2-[(phenylmethyl)amino]cyclohexyl]-, (αR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:531525 CAPLUS

DOCUMENT NUMBER: 117:131525

TITLE: Cycloaddition reactions of γ-amino α,β-didehydro amino acid esters: a test case for the principle of 1,3-allylic strain

AUTHOR(S): Reetz, Manfred T.; Kayser, Frank; Harms, Klaus

CORPORATE SOURCE: Max-Planck-Inst. Kohlenforsch., Muelheim/Ruhr, 4330, Germany

SOURCE: Tetrahedron Letters (1992), 33(24), 3453-6

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:131525

AB N,N-dibenzylamino aldehydes (PhCH<sub>2</sub>)<sub>2</sub>NCH<sub>2</sub>CHO (R = Me, PhCH<sub>2</sub>, Me<sub>2</sub>CH, Me<sub>2</sub>CHCH<sub>2</sub>, Me<sub>3</sub>CSiMe<sub>2</sub>OCH<sub>2</sub>), readily accessible from amino acids, can be converted into γ-N,N-dibenzylamino α,β-didehydro amino acid esters (Z)- and (E)-(PhCH<sub>2</sub>)<sub>2</sub>NCH<sub>2</sub>CH:C(NHCHO)CO<sub>2</sub>Et (I) without racemization. (Z)-I undergo stereoselective Diels-Alder reactions and 1,3-dipolar cycloaddn. with diazomethane, the sense of diastereoselectivity being opposite to that predicted by the conventional principle of 1,3-allylic strain.

IT **143250-68-4P**

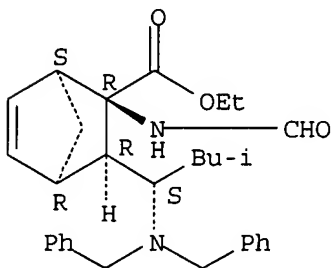
10/644,981

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 143250-68-4 CAPLUS

CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 3-[1-[bis(phenylmethyl)amino]-3-methylbutyl]-2-(formylamino)-, ethyl ester, [1S-[1 $\alpha$ ,2 $\beta$ ,3 $\beta$ (R\*),4 $\alpha$ ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:214485 CAPLUS

DOCUMENT NUMBER: 116:214485

TITLE: Preparation of 4-benzylisoxazoles as herbicides

INVENTOR(S): Cain, Paul A.; Cramp, Susan Mary; Little, Gillian M.

PATENT ASSIGNEE(S): Rhone-Poulenc Agriculture Ltd., UK

SOURCE: Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 8

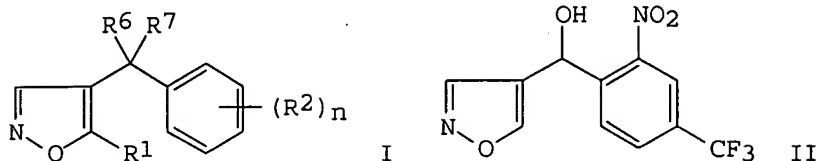
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 470856	A1	19920212	EP 1991-307351	19910809
EP 470856	B1	19951011		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AU 9181678	A1	19920213	AU 1991-81678	19910807
AU 643310	B2	19931111		
CA 2048705	AA	19920211	CA 1991-2048705	19910808
RO 109941	B1	19950728	RO 1991-148219	19910808
IL 99132	A1	19951231	IL 1991-99132	19910808
FI 9103782	A	19920211	FI 1991-3782	19910809
HU 58188	A2	19920228	HU 1991-2664	19910809
BR 9103433	A	19920519	BR 1991-3433	19910809
ZA 9106305	A	19921028	ZA 1991-6305	19910809
JP 05345770	A2	19931227	JP 1991-200537	19910809
AT 128972	E	19951015	AT 1991-307351	19910809
ES 2077806	T3	19951201	ES 1991-307351	19910809
RU 2055072	C1	19960227	RU 1991-5001315	19910809
CZ 282110	B6	19970514	CZ 1991-2473	19910809
CN 1058777	A	19920219	CN 1991-105623	19910810
US 5656573	A	19970812	US 1995-460093	19950602
PRIORITY APPLN. INFO.:			GB 1990-17539	A 19900810
			GB 1989-20519	A 19890911
			US 1990-580795	B2 19900911
			GB 1990-25469	A 19901122
			GB 1991-16833	A 19910805
			GB 1991-16835	A 19910805

10/644,981

US 1991-742381	B2 19910808
US 1991-790175	B2 19911112
US 1992-850031	B2 19920312
US 1992-850035	B2 19920312
US 1992-850128	B2 19920312
US 1992-850424	B2 19920312
US 1993-108792	B1 19930819

OTHER SOURCE(S): MARPAT 116:214485  
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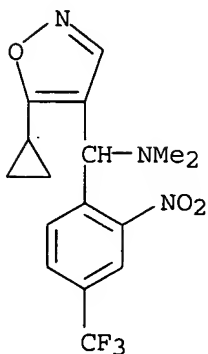
AB Title compds. I; R1 = (halo)alkyl, (halo)alkenyl, (halo)alkynyl, (substituted) cycloalkyl, cycloalkenyl, alkoxy carbonyl, aryl, aralkyl, amino, halo, CHO, etc.; R2 = NO<sub>2</sub>, cyano, halo, (halo)alkyl, alkylthio, alkylsulfinyl, alkylsulfonyl, sulfamoyl, alkoxy carbonyl, CHO, (thio)carbamoyl, alkoxy, alkoxyalkyl, etc.; R6 = H, OH, halo, (halo)alkyl, (halo)alkenyl, (substituted) cycloalkyl alkylthio, alkylsulfinyl, alkylsulfonyl, cyano, CHO, (thio)carbamoyl, alkoxy, PhO, PhCH<sub>2</sub>O, PhCO<sub>2</sub>, (acyl)amino, heterocyclyl, etc.; R7 = H (haloalkyl; R6R7 = (cyclic) (thio)ketal moiety; n = 1-5], were prepared. Thus, 4-(2-nitro-4-trifluoromethylbenzoyl)-5-cyclopropylisoxazole (preparation given) was reduced with NaBH<sub>4</sub> in EtOH to give title compound II. Numerous I at 1000 g/ha gave ≥90% reduction in growth of ≥1 weed.

IT 141111-96-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

RN 141111-96-8 CAPLUS

CN 4-Isloxazolemethanamine, 5-cyclopropyl-N,N-dimethyl-α-[2-nitro-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:157881 CAPLUS

DOCUMENT NUMBER: 112:157881

TITLE: 2-Hydroxy-3-aryloxypropylamine derivatives having cardiovascular activity

10/644,981

INVENTOR(S): Casagrande, Cesare; Santangelo, Francesco; Calabi, Maria Luisa  
PATENT ASSIGNEE(S): Societa Italiana Medicinali e Sintetici S.p.A. (SIMES), Italy  
SOURCE: Eur. Pat. Appl., 19 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 333938	A1	19890927	EP 1988-202681	19881124
EP 333938	B1	19930414		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 88176	E	19930415	AT 1988-202681	19881124
ES 2054790	T3	19940816	ES 1988-202681	19881124
US 5047425	A	19910910	US 1988-278205	19881130
JP 02000241	A2	19900105	JP 1988-305093	19881201
PRIORITY APPLN. INFO.:			IT 1987-22824	A 19871201
			EP 1988-202681	A 19881124

OTHER SOURCE(S): MARPAT 112:157881

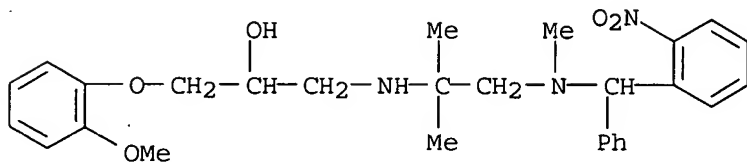
AB ArOCH<sub>2</sub>CH(OH)CH<sub>2</sub>NHCRR1XNR<sub>2</sub>(CH<sub>2</sub>)<sub>n</sub>CHR<sub>3</sub>R<sub>4</sub> [I; Ar = (un)substituted cyclic or bicyclic (hetero)aromatic group; R, R<sub>1</sub> = H, C1-3 alkyl; X = (CH<sub>2</sub>)<sub>p</sub>Y; Y = CH<sub>2</sub>, CO; p = 0, 1, 2; R<sub>2</sub> = H, C1-3 alkyl; n = 0, 1, 2; R<sub>3</sub>, R<sub>4</sub> = (un)substituted Ph] having β-blocking activity, thus useful as cardiovascular agents, e.g. in treatment of hypertension, angina pectoris, and heart arrhythmia, are prepared by (1) reaction of H<sub>2</sub>NCCR1XNR<sub>2</sub>(CH<sub>2</sub>)<sub>n</sub>CHR<sub>3</sub>R<sub>4</sub> with aryl glycidyl ether or ClCH<sub>2</sub>CH(OH)CH<sub>2</sub>OAr or (2) alkylation of ArOCH<sub>2</sub>CH(OH)CH<sub>2</sub>NHCRR1XNHR<sub>2</sub> with N(CH<sub>2</sub>)<sub>n</sub>CHR<sub>3</sub>R<sub>4</sub> (W = Cl, Br, MeSO<sub>3</sub>, p-Me(OH<sub>4</sub>SO<sub>3</sub>)). Thus, a solution of H<sub>2</sub>NCMe<sub>2</sub>CH<sub>2</sub>NMeCH<sub>2</sub>CHPh<sub>2</sub> and 1,2-epoxy-3-(2-methoxyphenoxy)propane in PhMe was refluxed 4 h to give, after silica gel chromatog. and acidification with HCl in EtOAc, 2-MeOC<sub>6</sub>H<sub>4</sub>OCH<sub>2</sub>CH(OH)CH<sub>2</sub>NHCMe<sub>2</sub>CH<sub>2</sub>NMeCH<sub>2</sub>CHPh<sub>2</sub>·2HCl. 2-MeOC<sub>6</sub>H<sub>4</sub>OCH<sub>2</sub>CH(OH)CH<sub>2</sub>NHCH<sub>2</sub>CHMeCH<sub>2</sub>NMeCHPh<sub>2</sub> had a high affinity towards the β<sub>1</sub> and β<sub>2</sub> receptors in guinea pig atria comparable to that of a known β-blocker, Propranolol.

IT 126059-35-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as β-blocker)

RN 126059-35-6 CAPLUS

CN 2-Propanol, 1-[[1,1-dimethyl-2-[methyl[(2-nitrophenyl)phenylmethyl]amino]ethyl]amino]-3-(2-methoxyphenoxy)-(9CI) (CA INDEX NAME)



L4 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:49955 CAPLUS

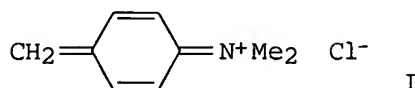
DOCUMENT NUMBER: 88:49955

TITLE: Photochemical studies on an aromatic amine-polychloromethane system. Part V. Mechanism of photochemical reactions in the system N,N-dimethylaniline-methylene chloride  
AUTHOR(S): Latowski, Tadeusz; Zelent, Bogumil



10/644,981

CORPORATE SOURCE: Inst. Chem., Univ. Gdansk, Gdansk, Pol.  
SOURCE: Roczniki Chemii (1977), 51(7-8), 1405-20  
CODEN: ROCHAC; ISSN: 0035-7677  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

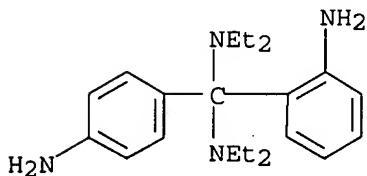


AB The mechanism of the photochem. reaction of PhNMe<sub>2</sub> with aqueous CH<sub>2</sub>Cl<sub>2</sub> involves the formation of PhNMe<sub>2</sub>+• and •CH<sub>2</sub>Cl (via an exciplex) which combine to form I which is autoxidized to give p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CHO. This mechanism was confirmed by the photoreaction of CH<sub>2</sub>Cl<sub>2</sub> with PhNEt<sub>2</sub>, Me(p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>)NPh, or (p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>CH<sub>2</sub>.

IT **65295-95-6P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 65295-95-6 CAPLUS

CN Methanediamine, 1-(2-aminophenyl)-1-(4-aminophenyl)-N,N,N',N'-tetraethyl-  
(9CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 17:46:24 ON 16 JUN 2005

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 178 S L1 FULL

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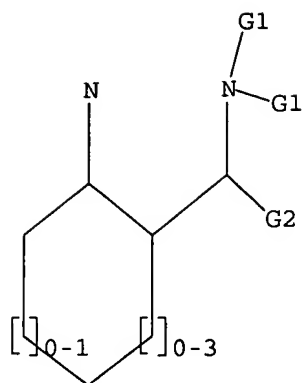
L4 12 S L3

=> d l1

L1 HAS NO ANSWERS

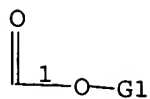
L1 STR

10/644,981



G1 Cb,Ak

G2 Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Cy,[@1]



Structure attributes must be viewed using STN Express query preparation.

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